Production of Phenol from Cumene - Systematic and Efficient Design Method

Bertran, Maria-Ona; Galvanin, Silvia; Mattei, Michele

Publication date:
2013

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Bertran, M-O., Galvanin, S., & Mattei, M. (2013). *Production of Phenol from Cumene - Systematic and Efficient Design Method*. Abstract from 2013 AIChE Annual Meeting, San Francisco, CA, United States.

330823 Production of Phenol From Cumene - Systematic and Efficient Design Method

Monday, November 4, 2013
Grand Ballroom B (Hilton)

Maria-Ona Bertran, **Silvia Galvanin** and Michele Mattei, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Kongens Lyngby, Denmark

Phenol (hydroxybenzene) is one of the most important intermediates of the chemical industry. It is the main feedstock for bisphenol A production, used to produce polycarbonate and epoxy resins. Phenol demand increases over the years and it is forecast to follow this trend, which, together with its wide range of applications, provides an excellent platform for the design of a sustainable process for phenol production.
A systematic hierarchical decomposition method is applied to design a sustainable plant for producing phenol, in which design decisions are made based on sustainability criteria. The process design work is divided into 12 sequential tasks that comprise all stages of conceptual design, starting from the consideration of qualitative aspects of the process flowsheet and preliminary calculations to detailed process simulations, equipment sizing, costing, economic evaluation, sustainability and LCA/sustainability assessment of the designed process. The design of the phenol production process is developed as part of the MSc-level course on Process Design at DTU.
As the base case design, auto-catalyzed oxidation of cumene to cumene hydroperoxide subsequently cleaved over a solid catalyst to phenol and acetone is selected. In this process, acetone is co-produced. Undesired formation of acetophenone and dimethyl benzyl alcohol, which dehydrates producing alpha methyl styrene, occur as side reactions. Alpha methyl styrene is hydrogenated back to cumene over a highly selective catalyst. The by-products and presence of azeotropes make the downstream separation of the products complex. Separation is done by a sequence of distillation units and phenol and acetone are obtained as pure products. In the first 2 tasks of the 12-tasks design procedure, information about the product and process is obtained. A modified Douglas approach is then used in task 3 to verify the selected process flowsheet from the literature. Tasks 4 to 8 include design decisions, mass and energy balances, rigorous simulation, and equipment sizing and costing. At the end of task 9, the economic analysis, the base case design is obtained, which is then further improved with respect to heat integration and process optimization. In the final task 12, a sustainability and LCA analysis is performed to assess the environmental impact of the process design. A commercial simulator is used for process simulation (design verification), ICAS for property prediction and analysis of design options and ECON for cost and economic evaluation.
A production rate of 300,000 metric tons/year of phenol is considered. In the base case, 0.66 kg of phenol and 0.41 kg of acetone are produced per kg of cumene with an energy consumption of 23,181 kJ/kg phenol. The base case design annual profit is estimated to be 50 million USD with a payback time of 2-3 years. Once the base case profitability has been determined, it is used as a reference to generate and analyze more sustainable alternatives. The targeted improvements are related to reduced energy consumption through better heat integration and process optimization, which results in identifying the more sustainable design in terms of raw materials usage, energy consumption, water consumption and environmental impact.

Extended Abstract: File Not Uploaded

See more of this Session: Poster Session: Systems and Process Design
See more of this Group/Topical: Computing and Systems Technology Division